

**Conformational Landscape, Infrared Characterization, and UV-Induced
Reactivity of 3-Chloromethyl-5-(3-Methoxyphenyl)-1,2,4-Oxadiazole
Isolated in a Nitrogen Matrix**

İsa Sıdır,^{1,2} A. J. Lopes Jesus^{3,*} and Rui Fausto^{2,4}

¹ *Department of Physics, Faculty of Sciences and Letters, Bitlis Eren University, Bitlis 13000, Türkiye*

² *University of Coimbra, CQC-IMS, Department of Chemistry, 3004-535 Coimbra, Portugal*

³ *University of Coimbra, CQC-IMS, Faculty of Pharmacy, 3000-548, Coimbra, Portugal.*

⁴ *Spectroscopy@IKU, Faculty of Sciences and Letters, Department of Physics, Istanbul Kultur University, Ataköy
Campus, Bakırköy 34156, Istanbul, Türkiye*

* Correspondence: ajorge@ff.uc.pt

1. Figures

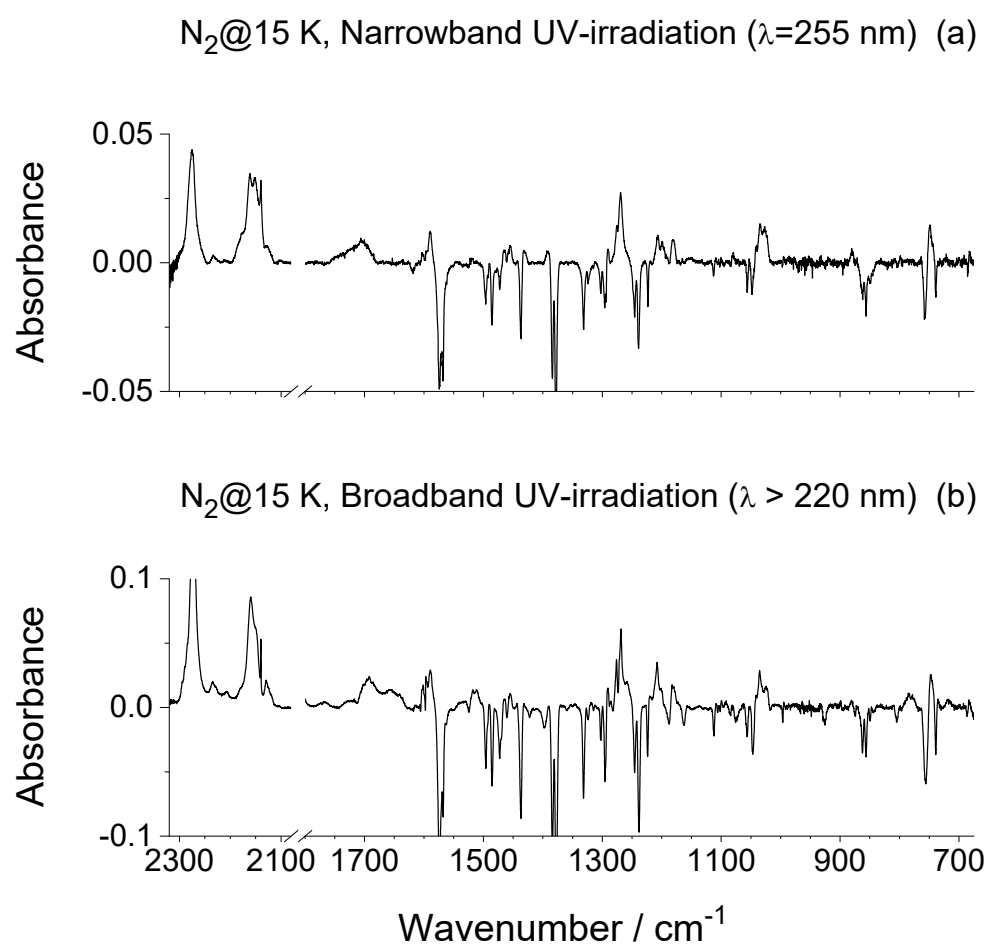


Figure S1. Comparison of difference IR spectra (N_2 , 15 K) in the 2320–675 cm^{-1} region following UV-irradiations: (a) spectrum obtained by subtracting the spectrum of the as-deposited matrix from that recorded after 60 min of narrowband UV irradiation ($\lambda = 255\text{ nm}$); and (b) spectrum obtained by subtracting the spectrum recorded after the narrowband UV irradiation from that recorded after an additional 6 min of broadband UV irradiation using a 500 W Hg(Xe) arc lamp, filtered through water ($\lambda > 220\text{ nm}$).

2. Tables

Table S1. DFT/B3LYP/6-311++G(d,p) calculated zero-point corrected energies for the conformers of CMPO (**1**) and putative photoproducts.^a

Molecule	Conformer	ΔE_0 / kJ mol ^{-1 a}	$\Delta E'_0$ / kJ mol ^{-1 a}	E_0 / Hartree ^b	
CMPO (1)	SASk	0.00		-1106.611167	
	SSSk	0.64			
	ASSk	2.30			
	AASk	2.47			
Isocyanate (2)	SA	-58.00 ^c	0.00	-514.264697	
	AA	-57.57 ^c	0.43		
	AS	-57.14 ^c	0.86		
	SS	-57.06 ^c	0.94		
2-Chloroacetonitrile (3)				-592.368561	-1106.63326 ^d
Carbodiimide (4)	SS	-54.42	0.00	-1106.631894	
	SA	-53.00	2.13		
	AS	-51.07	2.54		
	AA	-51.36	3.20		
Cyanamide (5) ^e	SSkAG	-48.18	0.00	-1106.62952	
	SGAG'	-47.71	0.47		
	SGAG	-47.25	0.92		
	SSkAG'	-46.67	1.51		
	AGAG'	-45.84	2.34		
	ASkAG	-45.32	2.85		
	AGAG	-44.95	3.22		
	ASkAG'	-44.82	3.36		
Diazirine (6) ^f	SSS	172.25	0.00	-1106.545560	
	SAS	173.07	0.82		
	AAS	175.41	3.16		
	ASS	175.46	3.21		
Nitrilimine (7) ^g	SSS	105.23	0.00	-1106.571086	
	SAS	106.58	1.34		
	AAS	108.20	2.97		
	ASS	108.36	3.12		
1,3,4-Oxadiazole (8)	SA	-24.08	0.00	-1106.62034	
	SS	-21.95	2.13		
	AS	-21.54	2.54		
	AA	-20.88	3.20		

^a ΔE_0 and $\Delta E'_0$ are the difference of zero-point corrected energies relative to the **CMPO (1)** most stable conformer and to the most stable conformer of the molecule, respectively. ^b 1 Hartree = 2625.5001 kJ mol⁻¹. ^c The given relative energy corresponds to the difference between the sum of the energies of **2** and **3** and that of the most stable form of **1**. ^d Sum of the zero-point corrected energies of **2** and **3** in Hartree. ^e Cyanamide **5** has eight additional high-energy conformers. ^f Diazirine **6** has eight additional conformers that are separated by very low energy barriers from the four conformers indicated in the table and that have energies higher than at least one of these latter, so expected to promptly decay into these if formed. ^g Nitrilimine has four additional high-energy conformers. For the structures of the lowest energy conformer of each putative photoproduct molecule, see the Figure 9). Conformers are labeled according to the torsional arrangements about selected bonds, as illustrated in Figure 9.

Table S2. B3LYP/6-311++G(d,p) calculated vibrational frequencies (ν/cm^{-1} ; scaled) and infrared intensities ($I^{\text{IR}}/\text{km mol}^{-1}$) for the most relevant conformers of **CMPO (1)** and for the most stable conformers of the observed photoproducts isocyanate (**2**) and 2-chloroacetonitrile (**3**).

1, SASk		1, SSSk		1, AASk		1, ASSk		2, SA		3	
ν	I^{IR}	ν	I^{IR}	ν	I^{IR}	ν	I^{IR}	ν	I^{IR}	ν	I^{IR}
3094	2.6	3094	1.7	3082	3.8	3083	3.7	3092	1.2	3017	0.7
3081	1.2	3082	1.4	3082	0.9	3080	0.3	3073	2.8	2966	3.7
3069	3.9	3069	3.8	3078	3.9	3079	4.0	3063	5.9	2267	0.4
3051	6.9	3051	7.2	3050	8.1	3050	8.3	3046	6.4	1433	7.3
3014	20.2	3014	20.0	3013	18.5	3013	18.4	3011	20.0	1277	25.9
3007	0.2	3007	0.1	3007	0.1	3007	0.2	2945	34.8	1183	0.8
2960	7.7	2961	7.4	2961	7.4	2961	7.4	2887	48.0	935	16.8
2948	32.2	2948	31.7	2944	34.8	2944	34.8	2263	1802.1	901	0.7
2889	41.1	2889	40.9	2886	54.8	2887	54.9	1605	273.3	714	36.8
1605	66.5	1609	39.1	1583	26.2	1619	10.1	1590	55.6	477	3.6
1603	62.2	1596	5.3	1562	128.8	1590	16.6	1516	41.2	347	0.2
1566	177.2	1571	309.6	1535	155.4	1568	346.0	1478	43.5	185	5.6
1527	8.1	1527	12.0	1496	3.7	1527	14.2	1474	48.1		
1481	61.5	1491	84.1	1445	27.5	1487	82.1	1463	9.6		
1473	101.0	1474	54.8	1445	98.7	1474	40.4	1442	29.3		
1464	10.2	1464	10.3	1434	9.7	1464	9.8	1420	1.4		
1457	3.7	1449	15.1	1425	38.1	1446	5.2	1326	29.6		
1440	23.5	1440	27.7	1411	34.7	1440	29.1	1278	0.1		
1433	66.6	1420	17.2	1410	62.6	1430	14.0	1254	206.0		
1364	59.8	1366	80.2	1336	61.8	1365	66.7	1179	4.2		
1337	48.7	1338	38.0	1304	18.2	1332	34.1	1160	9.6		
1294	68.2	1312	17.8	1270	148.1	1308	15.1	1144	0.6		
1285	87.5	1279	57.1	1249	27.6	1288	133.1	1112	60.4		
1246	60.3	1243	154.2	1222	30.1	1238	105.8	1079	9.7		
1229	160.5	1225	183.2	1200	213.2	1219	186.7	1040	55.7		
1179	0.5	1180	9.7	1155	0.5	1179	0.5	988	2.0		
1179	5.2	1179	0.5	1153	8.4	1178	14.8	954	0.1		
1164	4.1	1161	4.0	1149	1.3	1170	1.7	894	74.9		
1145	0.6	1144	0.6	1121	0.7	1144	0.7	863	0.1		
1112	21.2	1111	1.9	1079	29.7	1105	8.5	844	33.7		
1084	9.9	1074	17.4	1073	11.1	1083	29.3	767	38.6		
1040	55.1	1041	45.6	1028	95.8	1053	84.9	715	10.7		
1025	4.7	1022	4.8	1002	3.3	1022	3.0	680	22.8		
991	7.8	993	13.4	969	2.6	989	0.9	635	32.4		
985	1.0	988	0.6	963	1.8	987	2.7	600	0.8		
973	0.1	974	0.1	942	0.0	963	0.0	564	18.7		
918	2.5	918	2.6	900	2.1	918	2.2	552	6.6		
906	11.4	904	0.0	887	6.7	904	9.9	468	0.6		
901	0.1	903	13.1	877	14.8	893	12.2	450	0.3		
872	17.6	864	19.7	860	2.1	880	5.2	450	2.7		
848	40.2	856	43.8	818	24.4	842	25.6	374	2.1		
795	21.5	795	24.6	766	20.8	786	18.0	264	0.6		
777	65.0	775	60.9	761	68.2	775	65.8	237	0.1		
747	31.4	746	26.3	730	36.5	746	37.5	205	8.3		
700	10.4	697	6.5	687	14.0	699	3.4	198	0.1		
682	16.6	679	16.7	660	14.5	676	15.0	89	5.5		
668	1.8	670	2.4	656	0.7	674	7.3	79	1.1		

Table S2. Continued.

642	1.2	642	1.6	629	1.3	644	2.0	50	0.0		
572	0.6	569	0.5	559	0.6	569	0.5				
566	5.8	564	4.6	553	5.2	566	6.8				
489	0.2	483	3.4	507	2.2	512	4.3				
451	2.4	449	2.3	442	2.9	449	2.6				
446	1.1	441	0.6	434	2.2	418	0.6				
370	1.2	383	0.5	321	1.7	381	1.5				
328	1.1	329	1.0	320	1.0	328	1.0				
273	0.1	288	2.9	277	0.4	261	1.4				
262	1.2	262	1.2	256	0.8	261	0.8				
230	2.7	215	0.4	227	0.8	216	0.0				
213	0.4	199	1.2	207	2.6	209	3.1				
193	1.3	192	1.8	194	0.1	199	0.0				
146	1.2	158	0.2	149	0.4	162	0.6				
94	6.9	98	4.7	101	0.1	103	0.0				
87	0.1	85	0.7	67	0.4	71	4.3				
68	0.0	69	0.7	65	6.3	69	0.4				
41	0.7	38	3.3	41	1.6	37	3.1				
22	1.8	23	1.0	21	1.0	21	0.3				

Table S3. B3LYP/6-311++G(d,p) calculated vibrational frequencies (ν/cm^{-1} ; scaled) and infrared intensities ($I^{\text{IR}}/\text{km mol}^{-1}$) for the most stable conformers of observed and non-observed photoproducts carbodiimide (**4**), cyanamide (**5**), diazirine (**6**), nitrilimine (**7**) and 1,3,4-oxadiazole (**8**).

4, SS		5, SSkAG		6, SSS		7, SSS		8, SA	
ν	I^{IR}	ν	I^{IR}	ν	I^{IR}	ν	I^{IR}	ν	I^{IR}
3092	5.5	3096	0.7	3094	1.7	3091	6.5	3093	2.6
3087	0.8	3080	2.1	3091	5.0	3087	1.0	3079	1.9
3066	6.6	3078	5.9	3067	6.2	3065	8.5	3068	4.0
3048	7.6	3069	3.0	3050	7.2	3045	9.8	3050	6.9
3027	1.6	3052	6.0	3013	21.2	3015	1.7	3049	0.3
3012	22.0	3016	18.1	3010	2.5	3009	24.9	3014	21.2
2971	19.3	3004	5.7	2957	5.6	2964	2.8	2981	5.1
2948	32.4	2954	23.5	2948	32.1	2945	33.9	2950	30.9
2889	43.6	2892	36.2	2889	42.3	2888	45.5	2891	41.4
2164	2399.1	2244	114.3	1825	24.5	2266	1066.6	1606	80.7
1693	229.7	1735	324.8	1689	227.7	1667	172.9	1601	36.3
1602	103.5	1604	97.9	1601	96.7	1602	107.0	1566	15.3
1592	13.7	1590	22.8	1590	13.4	1592	31.4	1545	89.5
1488	13.6	1494	42.8	1487	32.3	1488	21.6	1480	49.7
1485	131.7	1475	60.1	1473	74.6	1474	69.6	1473	122.9
1473	91.4	1466	11.4	1464	10.1	1463	9.6	1464	10.3
1463	10.0	1455	0.7	1454	9.0	1454	9.9	1460	7.6
1454	24.3	1436	31.5	1428	78.8	1428	67.1	1437	11.9
1453	3.0	1425	31.4	1419	21.6	1423	15.4	1434	61.9
1427	95.8	1338	45.1	1341	76.4	1339	371.2	1356	26.0
1340	70.2	1331	15.6	1294	8.2	1335	60.8	1337	51.0
1307	40.5	1321	52.8	1289	0.1	1286	1.8	1290	3.3
1288	0.8	1297	12.0	1265	487.8	1265	466.8	1275	12.6
1261	637.8	1270	242.1	1207	120.0	1247	436.2	1261	171.6
1222	18.6	1217	392.9	1174	31.7	1208	315.0	1222	51.7
1200	248.4	1185	19.5	1172	23.2	1178	0.4	1178	8.4
1171	117.2	1176	59.7	1158	29.2	1173	100.6	1163	5.2
1156	69.8	1162	14.9	1145	0.6	1157	41.3	1157	7.1
1145	0.6	1145	0.7	1103	184.6	1145	0.6	1145	0.6
1082	8.6	1106	78.1	1082	6.4	1081	23.0	1101	23.6
1055	174.4	1080	83.6	1049	10.8	1068	147.8	1084	6.8
1031	274.1	1037	41.0	1026	97.1	1036	151.2	1042	55.0
989	9.9	989	6.1	989	7.0	990	6.6	1028	16.9
975	0.1	977	29.9	977	0.1	971	0.1	990	0.7
934	1.3	975	1.3	919	0.2	908	0.6	985	17.9
917	134.7	907	0.6	908	5.1	897	95.7	969	0.1
912	0.5	900	58.4	888	52.3	887	14.4	966	18.6
886	14.8	860	16.6	886	16.8	875	11.0	895	1.2
824	60.7	846	12.2	844	48.3	849	215.1	894	0.3
805	12.8	799	18.9	815	12.0	801	11.8	870	18.9
773	104.6	743	69.7	785	30.3	780	10.4	854	55.7
752	51.4	689	11.9	764	31.3	747	50.9	790	27.9
678	11.3	683	42.6	739	27.8	679	10.8	758	13.4
669	59.2	675	49.1	678	13.2	667	2.0	726	42.7
662	59.2	634	39.2	671	0.6	635	99.4	706	32.3
611	77.5	596	10.7	576	11.1	566	5.5	681	21.2

Table S3. Continued.

568	5.2	554	7.0	557	15.1	555	13.2	671	6.0
540	6.4	538	5.8	545	30.6	510	42.5	630	15.4
523	2.5	521	5.9	465	0.4	479	0.1	577	1.3
457	0.8	459	0.6	446	0.9	460	5.7	564	3.0
446	0.7	443	2.8	442	0.9	446	0.6	470	7.1
435	1.9	421	16.6	403	1.3	436	4.0	455	2.0
378	48.5	361	2.5	387	2.4	359	72.5	441	0.5
328	0.3	325	8.9	312	0.8	322	11.2	370	2.6
264	1.0	294	2.1	264	0.9	264	0.9	332	2.3
235	3.1	267	6.4	255	0.7	235	0.2	310	2.1
209	0.2	261	3.0	206	1.0	220	3.1	263	0.7
178	0.6	208	1.0	196	6.9	207	0.2	250	0.5
163	0.5	176	8.8	174	1.8	168	0.5	208	1.4
127	2.6	154	1.2	144	0.4	144	7.4	195	1.1
104	11.2	108	7.2	135	5.1	99	2.8	115	1.8
91	6.4	96	2.1	96	2.0	85	4.4	100	2.0
59	3.6	80	4.4	93	10.4	64	7.1	97	3.7
47	3.3	58	0.7	42	2.7	48	2.2	85	6.6
20	1.0	36	0.2	38	0.7	27	0.8	46	1.3
17	1.3	29	1.5	18	1.3	23	0.7	25	0.8

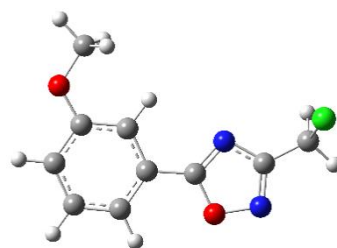
3. Computational data

Cartesian coordinates (Å) for the B3LYP/6-311++G(d,p) optimized geometries of the species described in this article.

CMPO (1)

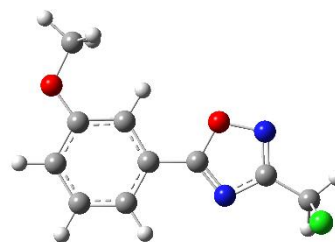
SASk

8	-1.104701000	-1.979949000	0.039314000
7	-2.463295000	-1.700272000	0.228350000
6	-2.476614000	-0.409379000	0.435158000
7	-1.244534000	0.190825000	0.403793000
6	-0.445332000	-0.810193000	0.156222000
6	1.006080000	-0.794068000	0.005894000
6	1.668235000	0.441041000	0.098233000
6	3.053269000	0.486907000	-0.041104000
6	3.771469000	-0.696388000	-0.270644000
6	3.104763000	-1.909570000	-0.359812000
6	1.718308000	-1.973438000	-0.223541000
8	3.795325000	1.624981000	0.028583000
6	3.126936000	2.862705000	0.252472000
6	-3.747531000	0.313905000	0.703093000
17	-4.222014000	1.366253000	-0.701014000
1	1.080346000	1.330429000	0.273510000
1	4.847889000	-0.635313000	-0.375869000
1	3.669616000	-2.817110000	-0.537984000
1	1.198631000	-2.919764000	-0.293725000
1	2.601176000	2.862703000	1.212834000
1	2.419031000	3.083740000	-0.552855000
1	3.907503000	3.620982000	0.267040000
1	-3.639756000	0.976805000	1.558482000
1	-4.557880000	-0.392028000	0.861802000



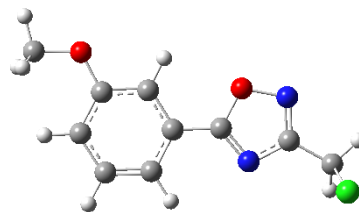
SSSk

8	0.620871000	-1.436816000	-0.182581000
7	1.991698000	-1.688766000	-0.317995000
6	2.501452000	-0.492944000	-0.460223000
7	1.588541000	0.529146000	-0.435676000
6	0.459438000	-0.099689000	-0.261359000
6	-0.884901000	0.457821000	-0.154161000
6	-1.989273000	-0.394342000	0.011857000
6	-3.266746000	0.153805000	0.112790000
6	-3.437325000	1.544219000	0.047677000
6	-2.337144000	2.374099000	-0.116055000
6	-1.052726000	1.842969000	-0.218144000
8	-4.404586000	-0.574620000	0.275264000
6	-4.303727000	-1.992788000	0.353913000
6	3.962572000	-0.296927000	-0.653112000
17	4.737424000	0.419850000	0.826486000
1	-1.830334000	-1.461801000	0.059113000
1	-4.440142000	1.945772000	0.128839000
1	-2.480708000	3.447243000	-0.163635000
1	-0.188272000	2.481285000	-0.343381000
1	-3.696537000	-2.301793000	1.211064000
1	-5.322085000	-2.354291000	0.483306000
1	-3.882657000	-2.413612000	-0.565090000
1	4.152133000	0.400604000	-1.465591000
1	4.450701000	-1.249352000	-0.839742000



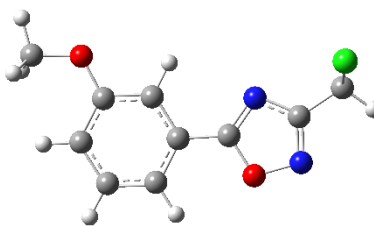
ASSk

8	0.813817000	-1.543509000	-0.103805000
7	2.196670000	-1.721121000	-0.224551000
6	2.637506000	-0.506444000	-0.424427000
7	1.666228000	0.460754000	-0.451098000
6	0.575628000	-0.224539000	-0.248025000
6	-0.798643000	0.262606000	-0.171005000
6	-1.854022000	-0.626889000	0.028310000
6	-3.165531000	-0.147811000	0.100305000
6	-3.413874000	1.222117000	-0.027485000
6	-2.345856000	2.101527000	-0.226512000
6	-1.041187000	1.639804000	-0.299825000
8	-4.125403000	-1.093159000	0.296288000
6	-5.484321000	-0.680789000	0.384313000
6	4.085442000	-0.235770000	-0.625236000
17	4.811192000	0.601253000	0.815898000
1	-1.679957000	-1.690143000	0.129756000
1	-4.421060000	1.612555000	0.025813000
1	-2.547231000	3.162118000	-0.323381000
1	-0.211234000	2.316913000	-0.451190000
1	-5.815281000	-0.197439000	-0.541004000
1	-6.059585000	-1.591336000	0.541023000
1	-5.641266000	-0.002592000	1.229730000
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1	4.628856000	-1.166614000	-0.761013000



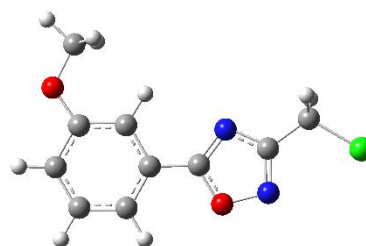
AASk

8	1.261896000	1.881873000	-0.008510000
7	2.620274000	1.604816000	0.182440000
6	2.631007000	0.321304000	0.432320000
7	1.397025000	-0.275770000	0.428098000
6	0.599947000	0.718185000	0.151796000
6	-0.853522000	0.707923000	0.010848000
6	-1.530890000	-0.501910000	0.159641000
6	-2.921634000	-0.543010000	0.031593000
6	-3.629616000	0.630859000	-0.247199000
6	-2.937749000	1.835443000	-0.394733000
6	-1.557755000	1.890202000	-0.269141000
8	-3.491348000	-1.768458000	0.194763000
6	-4.903773000	-1.888613000	0.073301000
6	3.900823000	-0.397821000	0.716247000
17	4.378872000	-1.473935000	-0.668487000
1	-0.988196000	-1.413599000	0.372705000
1	-4.706093000	0.620494000	-0.351075000
1	-3.494039000	2.740130000	-0.611053000
1	-1.027695000	2.826135000	-0.384624000
1	-5.244352000	-1.599145000	-0.926498000
1	-5.421844000	-1.285968000	0.826870000
1	-5.125767000	-2.941191000	0.238802000
1	3.789293000	-1.046021000	1.582262000
1	4.711367000	0.310047000	0.865063000



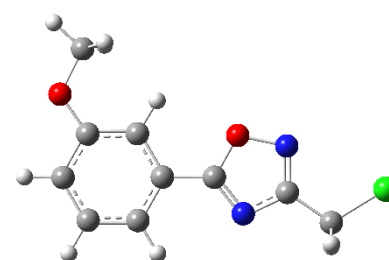
SAS

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7	1.207720000	0.133924000	0.000000000
6	0.000000000	0.629738000	0.000000000
6	-1.272616000	-0.085587000	0.000000000
6	-1.247602000	-1.489837000	0.000000000
6	-2.448217000	-2.195825000	0.000000000
6	-3.667047000	-1.500945000	0.000000000
6	-3.677463000	-0.113856000	0.000000000
6	-2.484582000	0.608638000	0.000000000
8	-2.541881000	-3.553419000	0.000000000
6	-1.342190000	-4.320283000	0.000000000
6	3.482982000	1.128219000	0.000000000
17	4.356149000	2.698172000	0.000000000
1	-0.289818000	-1.989778000	0.000000000
1	-4.587531000	-2.072067000	0.000000000
1	-4.624605000	0.412782000	0.000000000
1	-2.492932000	1.690488000	0.000000000
1	-0.742819000	-4.121412000	0.894461000
1	-0.742819000	-4.121412000	-0.894461000
1	-1.657693000	-5.361919000	0.000000000
1	3.797480000	0.575242000	-0.884537000
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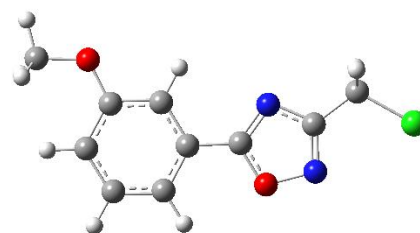
SSS

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7	-0.123339000	1.762026000	0.000000000
6	0.000000000	0.462919000	0.000000000
6	-1.051081000	-0.550228000	0.000000000
6	-0.711645000	-1.913307000	0.000000000
6	-1.724676000	-2.870670000	0.000000000
6	-3.067549000	-2.466618000	0.000000000
6	-3.388455000	-1.116446000	0.000000000
6	-2.388049000	-0.146093000	0.000000000
8	-1.511388000	-4.214445000	0.000000000
6	-0.170607000	-4.694481000	0.000000000
6	1.486754000	3.651060000	0.000000000
17	3.242492000	4.032394000	0.000000000
1	0.330565000	-2.197463000	0.000000000
1	-3.836509000	-3.229607000	0.000000000
1	-4.429663000	-0.815665000	0.000000000
1	-2.628360000	0.908730000	0.000000000
1	0.369243000	-4.367446000	0.894665000
1	-0.246035000	-5.780187000	0.000000000
1	0.369243000	-4.367446000	-0.894665000
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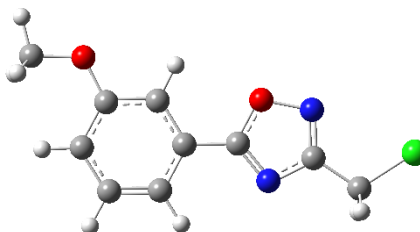
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6	0.000000000	0.649418000	0.000000000
6	1.031383000	-0.385152000	0.000000000
6	0.639390000	-1.723410000	0.000000000
6	1.604651000	-2.733556000	0.000000000
6	2.962696000	-2.398152000	0.000000000
6	3.340943000	-1.053398000	0.000000000
6	2.392912000	-0.041240000	0.000000000
8	1.123365000	-4.007216000	0.000000000
6	2.048335000	-5.088279000	0.000000000
6	-3.211124000	2.084324000	0.000000000
17	-3.620541000	3.833764000	0.000000000
1	-0.409467000	-1.989689000	0.000000000
1	3.725710000	-3.164634000	0.000000000
1	4.395245000	-0.802073000	0.000000000
1	2.692067000	0.998350000	0.000000000
1	2.679426000	-5.073474000	0.894928000
1	2.679426000	-5.073474000	-0.894928000
1	1.444311000	-5.993694000	0.000000000
1	-3.665024000	1.638545000	0.884454000
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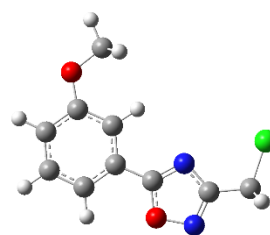
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6	-0.545409000	2.545709000	0.000000000
7	0.546890000	1.712023000	0.000000000
6	0.000000000	0.527327000	0.000000000
6	0.661758000	-0.774835000	0.000000000
6	-0.091444000	-1.948434000	0.000000000
6	0.551484000	-3.190065000	0.000000000
6	1.948282000	-3.250389000	0.000000000
6	2.690030000	-2.065717000	0.000000000
6	2.065034000	-0.828694000	0.000000000
8	-0.269666000	-4.275752000	0.000000000
6	0.312128000	-5.574192000	0.000000000
6	-0.348245000	4.027461000	0.000000000
17	-1.879089000	4.967892000	0.000000000
1	-1.173234000	-1.919984000	0.000000000
1	2.464478000	-4.200774000	0.000000000
1	3.772492000	-2.121571000	0.000000000
1	2.635580000	0.090372000	0.000000000
1	0.921658000	-5.738121000	0.894963000
1	-0.523178000	-6.271917000	0.000000000
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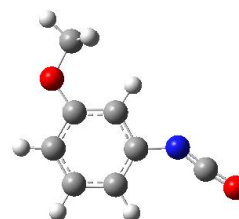
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7	1.33897800	0.02585300	0.00019800
6	0.46790200	-0.94832800	-0.00019500
6	-0.98811500	-0.85232500	0.00005500
6	-1.56698200	0.42729400	-0.00021300
6	-2.95432900	0.55054200	0.00004300
6	-3.75762600	-0.59982100	0.00057900
6	-3.17257800	-1.85772400	0.00084900
6	-1.78526500	-1.99937700	0.00058100
8	-3.62007700	1.73695400	-0.00018400
6	-2.86315700	2.94378400	-0.00082200
6	3.89609900	-0.00537300	-0.00008600
17	3.84463800	1.79117300	0.00072100
1	-0.91458300	1.28859400	-0.00060000
1	-4.83408700	-0.47847100	0.00077500
1	-3.80283900	-2.73934900	0.00127400
1	-1.32941200	-2.98061300	0.00079400
1	-2.23641900	3.01967000	-0.89522500
1	-2.23604100	3.02038200	0.89325400
1	-3.59406100	3.75018500	-0.00098900
1	4.45006700	-0.31270100	-0.88525800
1	4.45015000	-0.31348400	0.88476100



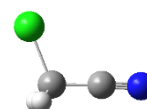
Isocyanate (2), SA

6	0.571625000	0.520930000	0.000000000
6	0.000000000	-0.757019000	0.000000000
6	-1.389482000	-0.886526000	0.000000000
6	-2.201267000	0.255382000	0.000000000
6	-1.615503000	1.512942000	0.000000000
6	-0.228812000	1.664049000	0.000000000
8	-2.043770000	-2.080877000	0.000000000
1	0.656949000	-1.614588000	0.000000000
1	-3.276746000	0.130716000	0.000000000
1	-2.246132000	2.394619000	0.000000000
1	0.223516000	2.648233000	0.000000000
7	1.970442000	0.598883000	0.000000000
6	2.848179000	1.421798000	0.000000000
8	3.784636000	2.124118000	0.000000000
6	-1.279555000	-3.280815000	0.000000000
1	-0.652232000	-3.354250000	0.894639000
1	-2.004249000	-4.093027000	0.000000000
1	-0.652232000	-3.354250000	-0.894639000



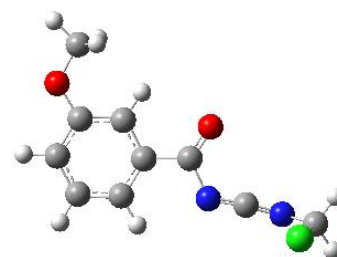
2-Chloroacetonitrile (3)

7	-2.305669000	-0.396424000	0.000000000
6	-1.279366000	0.127483000	0.000000000
6	0.000000000	0.817039000	0.000000000
17	1.390237000	-0.339408000	0.000000000
1	0.090927000	1.438889000	0.889356000
1	0.090927000	1.438889000	-0.889356000



Carbodiimide (4), SS

8	-0.303706000	-1.582272000	-0.489708000
7	-1.279148000	0.512482000	-0.639857000
6	-0.179425000	-0.377305000	-0.454213000
6	1.115230000	0.313310000	-0.220326000
6	2.251816000	-0.490741000	-0.036859000
6	3.488668000	0.106198000	0.186514000
6	3.589678000	1.505900000	0.226142000
6	2.461451000	2.291607000	0.043917000
6	1.215047000	1.704859000	-0.180856000
8	4.652411000	-0.575331000	0.377161000
6	4.617519000	-1.998425000	0.351507000
6	-4.782236000	-0.428267000	-0.477110000
17	-4.812437000	0.016538000	1.295891000
1	2.127667000	-1.563602000	-0.074956000
1	4.562962000	1.948529000	0.401612000
1	2.551806000	3.371211000	0.077252000
1	0.331334000	2.311490000	-0.322838000
1	4.276769000	-2.370787000	-0.620115000
1	3.971353000	-2.394968000	1.141450000
1	5.642167000	-2.322312000	0.524659000
1	-4.964275000	-1.500456000	-0.522543000
1	-5.603764000	0.114837000	-0.937282000
6	-2.433015000	0.136201000	-0.831134000
7	-3.569802000	-0.111665000	-1.137644000



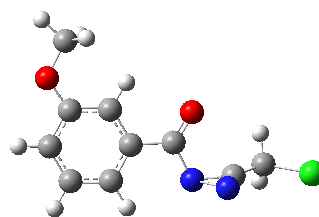
Cyanamide (5), SSkAG

8	-1.391303000	-2.194466000	-0.498728000
7	-1.685631000	-0.212961000	0.581616000
6	-0.854246000	-1.225280000	-0.019207000
6	0.617886000	-1.020630000	-0.003318000
6	1.199368000	0.241621000	-0.193838000
6	2.589516000	0.358952000	-0.230903000
6	3.388537000	-0.781651000	-0.073028000
6	2.801530000	-2.026289000	0.105753000
6	1.414951000	-2.159744000	0.130720000
8	3.254368000	1.528935000	-0.415556000
6	2.502460000	2.736688000	-0.519444000
6	-3.115439000	-0.276650000	0.365022000
17	-3.656785000	0.802981000	-0.997518000
1	0.577052000	1.113006000	-0.331601000
1	4.465168000	-0.664288000	-0.098491000
1	3.429601000	-2.901483000	0.223812000
1	0.947431000	-3.127919000	0.252242000
1	1.895429000	2.904254000	0.375408000
1	1.860732000	2.728857000	-1.406687000
1	3.238066000	3.532817000	-0.615295000
1	-3.643988000	0.055713000	1.252485000
1	-3.372103000	-1.291970000	0.084958000
6	-1.227039000	0.755495000	1.390459000
7	-0.891756000	1.600035000	2.107234000



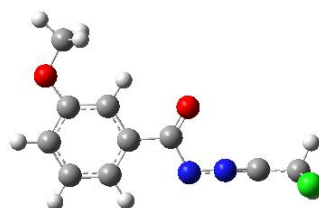
Diazirine (6), SSS

8	-0.644061000	-1.278386000	0.060576000
7	-2.446366000	0.856835000	1.167268000
6	-2.676686000	0.376325000	0.049623000
7	-1.385086000	0.921805000	-0.140350000
6	-0.363637000	-0.098210000	-0.015031000
6	1.021637000	0.425854000	-0.051128000
6	2.070823000	-0.508072000	-0.001283000
6	3.388527000	-0.063601000	-0.018336000
6	3.657991000	1.313216000	-0.085284000
6	2.616465000	2.227498000	-0.133290000
6	1.289296000	1.795538000	-0.118464000
8	4.479985000	-0.876267000	0.027149000
6	4.275953000	-2.283390000	0.103308000
6	-3.661080000	-0.342199000	-0.776236000
17	-5.238026000	-0.534037000	0.065324000
1	1.817305000	-1.557211000	0.054227000
1	4.692324000	1.635870000	-0.096565000
1	2.838385000	3.287184000	-0.183137000
1	0.471766000	2.501272000	-0.157168000
1	3.736581000	-2.655148000	-0.774063000
1	3.729413000	-2.557393000	1.011549000
1	5.270321000	-2.725088000	0.131392000
1	-3.267014000	-1.331659000	-1.007706000
1	-3.825596000	0.209794000	-1.702542000



Nitrimine (7), SSS

8	-0.389920000	-1.279238000	-0.451017000
7	-2.293744000	0.468132000	-0.558508000
6	-3.378947000	0.109702000	-0.765328000
7	-1.128346000	0.920724000	-0.388914000
6	-0.143875000	-0.091009000	-0.329719000
6	1.231062000	0.444052000	-0.111356000
6	2.277195000	-0.488074000	-0.043339000
6	3.582544000	-0.048666000	0.160111000
6	3.843338000	1.322683000	0.295364000
6	2.802056000	2.237287000	0.226616000
6	1.489377000	1.809351000	0.023150000
8	4.669169000	-0.869141000	0.241976000
6	4.469399000	-2.272130000	0.114856000
6	-4.751905000	-0.317935000	-0.716495000
17	-5.439736000	-0.341288000	0.983659000
1	2.030269000	-1.534610000	-0.152279000
1	4.866506000	1.642412000	0.453153000
1	3.014033000	3.295174000	0.332652000
1	0.675682000	2.519185000	-0.030931000
1	4.046817000	-2.527934000	-0.862445000
1	3.815459000	-2.655182000	0.905246000
1	5.456235000	-2.721595000	0.211648000
1	-4.842118000	-1.332158000	-1.102878000
1	-5.388185000	0.350087000	-1.295249000



1,3,4-Oxadiazole (8), SASk

7	-2.009170000	-1.824927000	-0.255600000
6	-2.514350000	-0.648378000	-0.428483000
6	-0.412791000	-0.373288000	-0.225051000
6	0.859642000	0.333604000	-0.153894000
6	2.030432000	-0.422356000	0.023835000
6	3.259979000	0.227031000	0.096394000
6	3.320853000	1.625271000	-0.008723000
6	2.157559000	2.359203000	-0.183278000
6	0.916928000	1.724872000	-0.257306000
8	4.452730000	-0.404944000	0.266950000
6	4.461926000	-1.824415000	0.385750000
6	-3.932261000	-0.294665000	-0.633699000
17	-4.635016000	0.572391000	0.807928000
1	1.945429000	-1.496730000	0.100789000
1	4.289185000	2.107059000	0.050735000
1	2.214015000	3.438696000	-0.261575000
1	0.010593000	2.300698000	-0.389804000
1	4.066458000	-2.301676000	-0.516703000
1	3.886313000	-2.154306000	1.256573000
1	5.506166000	-2.102705000	0.514848000
1	-4.506399000	-1.205903000	-0.772873000
1	-4.060856000	0.375586000	-1.481038000
8	-1.566770000	0.328283000	-0.425889000
7	-0.638092000	-1.649265000	-0.124040000

